DATE: May 2, 1974

TO : Potential Stanford University Collaborators with the DENDRAL Project

FROM : Carl Djerassi, Professor of Chemistry

SUBJECT: Availability of Facilities

During the preparation (December, 1973) of our grant application entitled "Resource Related Research: Computers in Chemistry" your research group expressed interest in utilizing our facilities (see below) for assistance in solving structure elucidation problems related to health sciences. I now wish to notify you, in my role as P. I. for this grant, that it was funded as of May 1, 1974, for a three year period, substantially as requested.

I want to make a few general comments before describing the facilities which will become available during the course of this grant. Our primary goals, as spelled out in our grant application, deal with bringing state-of-the-art techniques in mass spectrometry and computer science to bear on solving problems of molecular structure. We are not funded to act as a general service facility; we have neither the time nor the personnel to function in this manner. We hope to operate in a collaborative manner with each of you to help decide questions concerning the specific instrumental and computer techniques which can be brought to bear on your problems.

Facilities

A) Mass Spectrometry. Our primary goal is to provide the capability for routine gas chromatography/high resolution mass spectrometry. We will shortly receive a PDP 11/45 computer system for the laboratory which will be programmed to carry out this task. At the present time we can provide gas chromatography/low resolution mass spectrometry and severely restricted (without charge) access to high resolution mass spectra of single compounds as our budget provides only minimal funds for supporting this work pending the completion of the 11/45 data system. These facilities are available at no cost to the user.

B) Computer-Assisted Structure Elucidation. We have available a number of programs designed for automatic analysis of mass spectral data and also for isomer generation and manipulation and display of chemical structures. We are designing and programming interactive systems which will allow users to answer problems concerning the identity of molecular structures based on a variety of spectroscopic data. These interactive systems are under development, but are always available in their present state for tolerant users. These programs run on the SUMEX (Prof. Lederberg, P. I.) PDP-10 at the Medical School. Details of local user access are being worked out, but a significant amount of computer time will be available free of charge for users of these programs.

For the present time, those of you who are interested in making use of these facilities should contact (Med. School) Dr. Alan Duffield (Ext. 7-5788 (temporary, soon to be 7-6389) or (Chemistry Dept.) Dr. Dennis Smith (Ext. 7-3144). If serious bottlenecks occur, either with respect to the mass spectrometry laboratory or SUMEX, I intend to make use of an advisory committee described in our grant application to help rectify the problem. It is my hope that judicious selection of problems along the lines of the collaboration I outlined above will not make this necessary.

CD:ab

cc: Prof. J. Lederberg, Genetics
Prof. E. Feigenbaum, Computer Science